This is a resolution test chart (microfilm/microfiche target) containing the following numeric markings:

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4·5   1·8

1·25   1·4   1·6

Review of the Physics of Low-Dimensional Systems[†]

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Introduction

Over the past decade there has been considerable interest in the physics and chemistry of materials which exhibit highly anisotropic properties.[1] The crystals themselves are of course three dimensional, but in some cases the atomic or molecular arrangement is such that the electrons are constrained to move preferentially in only one or two directions and it is in this sense that the systems may be described as having reduced dimensionality. As we shall see in the following pages this reduced dimensionality has some unusual consequences which are responsible for the present excitement in this field.

One dimensional metals are, for example, intrinsically unstable against the formation at low temperatures of a variety of distortorted states. They may become magnetic or non-magnetic insulators or possibly even superconductors. The instabilities arise from the response of the system to weak perturbations. As the temperature is lowered we will find that the response "blows up." On the other hand we shall see that truly one-dimensional system cannot undergo phase transitions at any temperature above absolute zero. It is this apparent contradiction: that the system is unstable against a distortion but cannot

distort, that makes these studies fascinating. The resolution of the problem finally lies in the actual 3-dimensional nature of the crystals.

In addition, one-dimensional systems are interesting because some calculations which can be done only approximately in three dimensions can be done exactly in one dimension. Probably most important, there is a general feeling that it is potentially easier to use the apparatus of organic chemistry to synthesize properties that we want in one-dimensional compounds than in three-dimensional compounds.

Instabilities

When we talk about a system being unstable we mean that a small perturbation will evoke a large response. If we consider a system which contains many electrons in equilibrium and we then slightly change the potential they experience, the result will be a change in the electron wavefunctions and hence a change in the electron density. We will characterize the density change by a response function X_q^2 which gives the proportionality between the amplitude of a periodic potential $V(r)$ and the amplitude of the density change

$$\delta\rho(r) = X_q V(r) \qquad\qquad I$$

X_q is called a linear response function and it depends on how rapidly the potential is varying in space through the wavevector q (which is just $\frac{2\pi}{\lambda}$ λ being is the wavelength or period). In figure I we have illustrated the effect of an attractive interaction of the form $V(r) = V_o \cos \vec{q}\cdot\vec{r}$. In the absence of this potential the initial electron density is uniform. The potential is applied and the electrons move to regions where the attraction is large and away from regions where it is small or repulsive. The difference between the initial and final electron density is the response to the potential and has the same spatial dependence as the applied potential.

To place these abstract ideas on more realistic grounds we note that the energy of an electron with spin up in a magnetic field H is $-\mu_o H$ while that of an electron with spin down is $+\mu_o H$, where μ_o is the magnetic moment of the electron. The total magnetic moment of a collection of electrons is the number with up spins times μ_o plus the number of down spins times $-\mu_o$ or

$$M = \mu_o (\rho\uparrow - \rho\downarrow) \qquad\qquad II$$

Without a magnetic field the number up and down are equal so that M = 0. If we put on a magnetic field that varies with position we have

$$\delta\rho\!\uparrow = -X_q(-\mu_oH) \text{ and } \delta\rho\!\downarrow = X_q(\mu_oH)$$

$$M = \mu_o(\delta\rho\!\uparrow - \delta\rho\!\downarrow) = 2\mu_o^2X_qH \qquad\qquad III$$

The ratio of M to H is the magnetic susceptibility and we find it equal to $2\mu_o^2X_q$. If X_q diverges (goes to infinity) for some value of q then we have some problem in understanding equation III. It does not mean that a small magnetic field will give us an infinite total magnetic moment. Rather, it implies that with no magnetic field we have a finite total moment. For instance if $X_q \to \infty$ for $q \to o$ (which corresponds to very long wavelength or a uniform magnetic field), then we have a uniform magnetic moment with no applied field and this is the familiar case of a ferromagnet. If $X_q \to \infty$ for some other q then the magnetic moment varies with position and we have an antiferromagnet.

If we look instead at an electric field the energy of an electron is just its charge e times the potential ϕ. The total charge distribution Q in a metal is e times the electron density ρ plus the positive charge of the ions in the background. With no electric field Q = 0.

Putting on a spatially varying electric field we have

$$\delta Q = e\delta\rho = e\, X_q\, e\, \phi = e^2\, X_q\, \phi \qquad\qquad IV$$

If for some value of q, $X_q \to \infty$ the system is unstable against the formation of a periodic charge density. To make further connection with electromagnetic theory we note that a charge density produces itself produces a potential according to Maxwell's Equations so that

$$\nabla^2(\phi_1) = -4\pi e\delta\rho \qquad\qquad V$$

and using this expression we can relate the dielectric constant $\epsilon(q)$ to our response function

$$\epsilon(q) = 1 + \frac{4\pi e^2}{q^2} \, X_q \qquad\qquad VI$$

Naturally, the reason is we are going through all of this is that X_q does diverge for the one-dimensional systems we are interested in. The actual form of X_q for electrons in a metal is known as the Lindhard function and is given by:[3]

$$X_q = \sum_k \frac{f(k) - f(k + q)}{\epsilon_{k+q} - \epsilon_k} \qquad\qquad VII$$

Here we are summing over the different values of wavevectors k (or momentum ℏk) for the electron. f(k) is the Fermi-Dirac distribution function (and contains the interesting temperature dependence) and ϵ_k is the energy of the electron with momentum ℏk.

The Lindhard function is sketched as a function of q for one and three dimensional cases in figure 2. For one dimension there is a peak at a value of q equal to twice the Fermi wavevector. This peak increases as temperature is lowered, diverging logarithmically as $T \to 0$. For three dimensions there is no such peak. Understanding the origin of this peak is then essential to our study.

In order to proceed we have to remember a few simple results of quantum mechanics and what we have learned about electrons in metals from Prof. Garito's talk earlier in this conference. In the simplest case we can view the electrons in a metal as being "free" so that their only energy is kinetic. The wavefunctions are then

$$\phi_k = e^{i \vec{k} \cdot \vec{r}} \qquad\qquad VIII$$

and the energies are

$$\epsilon_k = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \qquad\qquad IX$$

We now apply a periodic potential of the form $V(r) = V_o \cos \vec{q} \cdot \vec{r}$. This perturbation will couple electrons whose wavevectors differ by $\vec{q}$. The wavefunctions for the electrons ψ_k will then be a combination of the original plane waves ϕ_k plus a little bit of the plane wave which is mixed in by the perturbation [4]

$$\psi_k \approx \phi_k + \frac{\langle \phi_{k+q} | V(r) | \phi_k \rangle \phi_{k+q}}{\varepsilon_{k+q} - \varepsilon_k} \qquad \text{X}$$

This is very similar to what happens when musical notes are mixed. We obtain additional tones at the sum and difference of the original tones. In our case only one of the additional frequencies is important. The amount of the mixing depends on how strongly the two wavefunctions are coupled divided by the original energy difference between the wavefunctions. This is known as perturbation theory in physics and as "configuration interaction" in chemistry. The density change which this brings about is just the density with the perturbation minus the original density

$$\rho = |\psi^2| - |\phi|^2 \approx \frac{V_o}{\varepsilon_{k+q} - \varepsilon_k} \cos \vec{q} \cdot \vec{r} \qquad \text{XI}$$

As expected we find that the density change is proportional to the applied periodic potential. If we want to know how the energies of the electron change, the general result is that the energies are pushed apart by the interaction that couples them. The additional splitting is equal to the coupling squared divided again by the energy difference.

$$\delta\varepsilon_k \approx \frac{V_o{}^2}{\varepsilon_k - \varepsilon_{k+q}}$$

$$\delta\varepsilon_{k+q} \approx \frac{V_o{}^2}{\varepsilon_{k+q} - \varepsilon_k} = -\delta\varepsilon_k \qquad \text{XII}$$

This is illustrated in figure 3a. Now if the states which are coupled have the same energy the energy denominator goes to zero and the expressions in X-XII diverge. This seems to give us the result we are looking for, but unfortunately it is not correct. Equations X-XII are only valid if the denominator is much larger than the numerator. In fact the largest the ratio $V_o/(\varepsilon_{k+q} - \varepsilon_k)$ can legitimately get is unity. This in fact is the result of the degenerate perturbation theory we must use. When we couple states with the same energy they are split by the coupling as illustrated in figure 3b. This of course is the origin of the "bonding and antibonding orbitals" which occur throughout organic chemistry.[4]

The electrons which have the same energy and are coupled by $V(r)$ are those with $k = -q/2$ and $k + q = q/2$. The wavefunction for the lower energy state is then

$$\psi_h = \frac{e^{i\frac{\vec{q}\cdot\vec{r}}{2}} + e^{-i\frac{\vec{q}\cdot\vec{r}}{2}}}{\sqrt{2}} = \sqrt{2}\ \cos\frac{\vec{q}\cdot\vec{r}}{2} \qquad \text{XIII}$$

$$\delta_\rho = \cos\vec{q}\cdot\vec{r}$$

Note that the density change has the same spatial dependence as $V(r)$ but there is not any dependence on how big the perturbation is (i.e., V_o does not appear in XIII). Thus for an infinitesimal perturbation we get a finite response. As advertised this is the true meaning of a divergent response function. If the states $q/2$ and $-q/2$ were both filled (with two electrons each) we would have no effect as both bonding and antibonding orbits would be filled after the perturbation is applied. Similarly if both are empty we have no effect. The cases of interest are states which are partially but not completely filled with electrons. Let us see how the states are occupied in a metal.

In figure 4a we see the situation for a three dimensional metal at low temperatures. The states with low kinetic energy are filled until we have accounted for all of the electrons in the metal. The momentum of the last electron added is called the Fermi momentum k_F and its energy, the Fermi energy ϵ_F. States with $|k| < k_F$ are filled and those above are empty.[5] For a particular value of q there are just two states which are connected by q which have the same energy and are partially filled (i.e., lie on the surface of constant ϵ_f, called the Fermi surface). Slightly different values of q will couple other states and give a density change with a different periodicity. Adding random periodicities results in no net contribution to the charge density.

By contrast we look at the situation for a one-dimensional metal (figure 4b). In one dimension the energy is determined solely by the momentum in one direction, call it $p_x = \hbar k_x$. All k states are occupied up to $|k_x| = k_f$. For any particular value of q, the states connected do not lie on the Fermi surface. However for $q = 2k_F$ there are many states which are connected by q and lie on the Fermi surface which in this case is just two parallel planes at $k_x = -k_F$ and $k_x = k_F$. The difference between one and three dimensions merely lies in the shape of the Fermi surface.

From these illustrations it is clear that the divergence we are looking for comes from having a plane of degeneracy, i.e., a vector $\vec{q}$ which will bring part of the Fermi surface into coincidence with another part. If one part of the Fermi surface fits into another part in this way we say the Fermi surface "nests." We will _always_ have Fermi surface "nesting" in one dimension since the Fermi surface is a set of parallel planes. Sometimes we can have a similar occurrence in two or three dimensions. As we have seen from Prof. Garito's lecture the free electron approximation is not always applicable.

For example if we have a three-dimensional metal described by tight binding bands the electron energies are given by:

$$\varepsilon_k = 2\tau_x \cos k_x a + 2\tau_y \cos k_y b + 2\tau_z \cos k_z c \qquad \text{XIV}$$

where the τ's are overlap integrals in each direction and a,b and c are the unit cell parameters. The Fermi surfaces are shown in figure 5 for a situation with one electron per unit cell. In this circumstance a wavevector $q = (\pi/a, \pi/b, \pi/c)$ will bring one part of the Fermi surface into coincidence with another part and the response function will diverge for this value of q.[6] We will see how these considerations effect the properties of transition metal sulfides in the following talk.

Kohn Anomaly

We would now like to investigate the kind of instabilities which result from the divergence of the response function. Up to this point we have neglected the ions which make-up the crystal in order to study the electrons. Suppose that the ions have a periodic displacement from their equilibrium position which has periodicity q and amplitude U_q. This is illustrated in figure 6.

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$$U_i = U_q \cos \vec{q} \cdot \vec{r}_i$$

Here U_i is the displacement of the ion at position r_i from its equilibrium position. Since the ions are charged, the displacement creates a periodic electrostatic potential on the electrons which we write as:

$$V(\vec{r}) = g U_q \cos \vec{q} \cdot \vec{r} \qquad \text{XVI}$$

g is a constant which relates the ion displacement to the electron potential and depends on the charge distribution on the ion.

The electrons will respond to this potential according to the χ_q we have just developed

$$\delta_\rho = X_q \ V(\vec{r}) = X_q \ g \ U_q \cos \vec{q} \cdot \vec{r} \qquad \text{XVII}$$

The electron charge density builds up in the region of positive charge created by the ions. The negative electrons in turn produce a force on the ions which tends to displace them further. The force in the direction of the original displacement is the same proportionality constant g as for the force of the ions on the electrons.

$$F = g\delta\rho \qquad \text{XVIII}$$

The magnitude of the force is then:

$$F = g^2 X_q U_q \qquad \text{XIV}$$

The periodic displacement of the ions is opposed by the elastic forces which hold the ions in place. The equation of motion for the displacements is usually written as

$$M \ \frac{d^2 U_q}{d\tau^2} = - K_q U_q \qquad \text{XX}$$

where M is the ion mass and K_q is the restoring force. This is just a complicated way of writing ma = F for a simple harmonic oscillator. If we assume that the displacements will vary simusoidally with time, the frequency of oscillation $\omega_o(q)$ is given by

$$- M \ \omega_o^2(q) \ U_q = - K_q U_q \qquad \text{XXI}$$

$$\omega_o(q) = \sqrt{K_q/M}$$

This equation gives the frequency as a function of wavevector for the lattice vibrations of a solid.[7] It is shown schematically as the solid line in figure 7. The dependence on q comes from the fact that if the crystal as a whole is displaced there is no restoring force (q = o) while if nearest neighbors ions (q = π/a) are moved in opposite directions the restoring force is a maximum.

We now add in the force due to the electronic response.

$$- M \omega^2(q) U_q = - K(q) + g^2 X_q U_q$$

$$\omega^2(q) = \frac{K(q)}{M} - g^2 \frac{Xq}{M} \qquad\qquad XXII$$

$$\omega^2(q) = \omega_o^2(q) - g^2 \frac{X_q}{M}$$

The lattice vibration frequencies are lowered by the interaction with the electrons. For a one-dimensional metal we have seen that X_q for $q = 2 k_F$ diverges as temperature is lowered. The frequency of this mode then decreases and goes to zero for some temperature above $T = 0$. This is illustrated by the dotted lines in figure 7.

The energy needed to create a periodic lattice displacement is $\hbar\omega$. If $\omega(q = 2k_F) = 0$ then a displacement at this period cost no energy and lasts forever (its frequency is zero) which implies a lattice distortion or crystal structure change.

We have therefore shown that a one-dimensional metal is unstable at some non-zero temperature against a crystal structure change with new periodicity of $q = 2 k_F$

Experimentally this "softening" of the lattice vibration frequency at $2 k_F$ has been seen in several systems which you will hear about at this conference. The effect was first predicted by Kohn and is known as a Kohn anomaly.[8]

Unfortunately our treatment so far does not tell us what happens after the distortion occurs. To see that, we return to look at the electrons using a description first presented by Peierls.[9]

Peierl's Transition

In figure 8 we have sketched the energy versus wavevector relationship for electrons in a metal. In the presence of a periodic potential $V_o \cos \vec{q} \cdot \vec{r}$, the states k and $k \pm q$ are mixed. As we have seen in figure 3 the energy levels repel one another and the shifts are given by eq. XII. Of course the shift can never exceed the result that we found in the degenerate limit. If we look at a level with momentum k as shown in figure 8 it mixes with $k-q$. The energy corresponding to k is lowered below its unperturbed value, while the energy of $k-q$ is increased. As k increases toward $\frac{q}{2}$ the energy is lowered even more as the energy difference between k and $k-q$ is getting smaller. The maximum energy lowering occurs when $k = q/2$ and the shift is V_o. Correspondingly $k-q$ is shifted up by V_o.

The energy vs. k after the potential has been added is shown in figure 9. There is now a region in which no allowed energies are to be found i.e., an energy gap. Note that all states with $|k| < q/2$ have lower energy than previously. If $k_F = q/2$ then the states filled with electrons have lower energy whereas the states which have higher energy are empty and thus do not contribute anything. The amount of electronic energy which is gained is represented by the shaded area in figure 9. This electronic energy lowering may be directly calculated and is equal to

$$\Delta E_e = - \frac{1}{2} N(E_F) V_o^2 (\frac{1}{2} + \ln (\frac{2\varepsilon_F}{V_o})) \qquad \text{XXIII}$$

where ε_F is the Fermi energy and $N(\varepsilon_F)$ is the density of states (number of electrons which had energy ε_F) before the perturbation was applied.

If the periodic potential is caused by a lattice displacement

$$V_o = gU_q$$

The elastic energy lost in causing this displacement is

$$E_L = \frac{1}{2} \ K_q U_g^{\ 2} \qquad\qquad \text{XXV}$$

as work is done against the restoring force of the ions.

The total energy change in distorting the lattice and opening the energy gap is:

$$E = E_2 + E_e = \frac{1}{2} \ K_q U_q^{\ 2} - \frac{1}{2} \ N(\epsilon_F) \ g^2 U_q^{\ 2} (\frac{1}{2} + \ln(\frac{2\epsilon_F}{gU_q})) \qquad\qquad \text{XXVI}$$

For small distortions the logarithmic term dominates as when $U_q \to 0$ $\ln(\frac{2\epsilon_F}{gU_q}) \to \infty$. The total system always has lower energy with a small distortion. The total energy is at a minimum when

$$gU_q = V_o = 2 \ \epsilon_F \ \exp\left[\frac{-K_q}{g^2 N(\epsilon_F)}\right] \qquad\qquad \text{XXVII}$$

So we have calculated the amplitude of the displacements and the size of the energy gap.

We might expect this energy lowering and distortion from any metal. Why is it a one-dimensional effect? The only electrons which are effected by the distortion are those connected by the wavevector q and within an energy range V_o of the Fermi energy. (This last statement is clear when we look at the energies in figure 9). For one dimension the electrons effected lie in the shaded area in figure 10 a . This fraction of electrons is V_o/ϵ_F. Each electron in this region has its energy lowered. Those which were at ϵ_F are lowered by V_o, those which were at $\epsilon_F - V_o$ are lowered only slightly. The average energy lowering is then $V_o/2$. For 1-dimension the total lowering is the number of electrons effected times their average energy gain or:

$$\text{1-dim} \qquad \Delta E_e \approx \frac{V_o^{\ 2}}{2\epsilon_F} \qquad\qquad \text{XXVIII}$$

In two dimensions the fraction of electrons effected by the opening of the gap is just the shaded slice in figure 10 b . The fraction of electrons effected is then approximately $(\frac{V_o}{\epsilon_F})^2$ and the average energy gain is $V_o/2$. For 2-dimensions the total lowering is then

$$\text{2-dim} \qquad \Delta E_e \simeq \frac{V_o^3}{2\epsilon_F^2} \qquad\qquad\qquad \text{XXIX}$$

If we performed the calculation more correctly we would have a logarithmic factor as in eq. XXVI. The elastic energy is the same for one or two dimensions. The total energy change upon undergoing a distortion is then

$$\text{1-dim} \qquad \Delta E = AV_o^2 - BV_o^2 \ln \left(\frac{E_f}{V_o}\right)$$

$$\text{2-dim} \qquad \Delta E = AV_o^2 - BV_o^3 \ln \left(\frac{E_f}{V_o}\right) \qquad\qquad \text{XXX}$$

For small values of V_o the second term in the 2-dimensional case is smaller than the first since $V_o \ln \left(\frac{E_f}{V_o}\right)$ goes to zero as V_o goes to zero.

We must remember however that if the Fermi surface "nests" in two or three dimensions then the situation looks very much like the one-dimensional cases. In fact when Peierls did his original calculation of this effect it was largely to explain why all metals were not in close packed structure. The point is that a distortion is always favorable in one-dimension and is sometimes favorable in 2 or 3 dimensions.

It is also noteworthy that the development of a gap at the Fermi surface of a one-dimensional metal will impede its conductivity (with some exceptions) and we therefore expect a metal insulator transition.

Phase Transitions

We have found that a metallic one-dimensional chain which would have a uniform charge density at high temperatures (figure 11a) is unstable against the formation of a distorted lattice and associated charge density wave at low temperature (figure 11b). This process may be regarded in simple chemical terms. When the ions distort from a uniform arrangement the charge density accumulates in the region where the ions are closest together essentially creating a chemical bond. The energy of the bond is the energy gap which has been opened, V_o.

Starting from low temperatures we would expect the bonds to be stable. As temperature is increased more of the bonds are broken or more electrons are excited across the energy gap. This lowers the energy of the distorted state relative to the uniform state. We would then expect the distortion to decrease until, at a temperature where the thermal energy is about equal to V_o we would return to the undistorted state. If the excitations or broken bonds are treated on the average (in "Mean Field Theory") we find the mean field transition temperature is relative to V_o by[10]

$$kT_{MF} = \frac{V_o}{1.76} \qquad \qquad XXXI$$

At this temperature we expect a distortion and gap to form and increase to a maximum value as temperature is lowered toward $T = 0$. This temperature dependence is sketched as the outer line in figure 12. We would assume that for $T < T_{MF}$ the system is completely ordered and the distortion just increases in amplitude. This is not the case.

Let us see what happens if we skip a lattice site when the distortion occurs. In figure 11b we saw the fully ordered phase. In figure 11c we see the order broken by a missed bond. What has happened in this picture is

that the ions have paired together up to site i. At this site the next atom
moved in the opposite direction rather than toward i. After this mistake the
ions are again paired. We have two fully ordered regions which meet at
point i. But the two regions are not ordered with respect to one another.

The energy difference between the phase with complete order and broken order
is simply the energy lost by the two electrons in the missing bond $2V_o$. The
break can be at any of N places along the chain to give us broken order, where
N is the number of sites along the chain. Since there are N ways the break
can occur the associated entropy in $k_B \ln N$. Now for finite temperatures we
should really be using the Helmholtz free energy which is internal energy
minus the temperature times the entropy. The free energy difference between
the ordered and broken phases is:[11]

$$\Delta F = 2V_o - k_B T \ln N \qquad\qquad \text{XXXII}$$

For a large system $(N \to \infty)$ the broken state is always favorable for any
temperature above absolute zero. This merely reflects the large number of
possible sites for a break.

The result we have found indicates that for temperatures above zero we
will have ordered regions separated by breaks. As temperature is raised
from zero there will be more breaks and the average size of the ordered
regions will decrease. If a chain has a small number of sites N it may still
remain ordered according to eq. XXXII up a certain temperature. The average
number of sites that will remain ordered at a temperature T is then obtained
by setting $\Delta F = 0$ [12]

$$N_{av.} = \exp \left(\frac{2V_o}{k_B T} \right)$$

Since the average distance between sites is the interatomic spacing a,
the length of this chain segment will be $(N_{av.})$ a. The average size of the
ordered regions is known as the correlation length and is written:

$$\xi\,(T) \;=\; a \, \exp \, (\frac{2V_o}{k_B T}\,) \qquad\qquad XXXIV$$

We again must ask why the situation is different for one dimension than
for two or three. In figure 13 a we have drawn several chains and assumed
that they interact with a two-dimensional electrostatic coupling. The
charge density on each chain has large negative charge on a bond and less
negative charge between bonds. Each bond would therefore like to see an
anti-bond at the appropriate position on each chain surrounding it. This
will occur if nearest neighbor chains have their charge density waves slipped
by one bond as in the illustration. We can represent the interchain
interactions by a (negative) term B which is added if a bond is adjacent to
antibond and subtracted if two bonds or two antibonds are adjacent.

In figure 13 b we have shown the situation with a broken bond in one
of the chains. In this case we not only lose the bond energy $2V_o$ as in one
dimension, but we have a repulsive interaction between the chains out to
the end of the crystal (which is about $\frac{N}{2}$ sites away if the break is toward
the center of the crystal). Thus we lose an addition $\frac{2BN}{2}$ in energy. The
difference in free energy between the ordered and broken states in figure 13
is then

$$F \;=\; 2V_o \;+\frac{2BN}{2}\; - \; k_B T \, \ell n(N) \qquad\qquad XXXV$$

For a large system $(N \to \infty)$ the second term dominates and the ordered phase
is stable below some temperature but above absolute zero. Thus in two
dimensions (or more) it is possible to have real phase transitions to ordered
states.

In any real systems there is always some three dimensional coupling between
the chains and this accounts for the phase transitions that are observed in

the "one-dimensional systems" which will be discussed in the following talks.
We can find the transition temperature by seeing what temperature will stabilize
the ordered state in eq. XXXV given a certain size for the system (number
of bonds in an ordered chain). This will occur on average when $\Delta F = 0$. The
number of bonds in an ordered chain is given on average by eq. XXXIII and is
itself temperature dependent.

We find:

$$0 = BN(T_c) - k_B T_c \, \ell n (N(T_c))$$

or   XXXVI

$$k_B T_c = \frac{2V_o}{\ell n (\frac{2V_o}{B})}$$

This expression uses the model depicted in figure 14 where each chain has
two nearest neighbors. If there are z nearest neighbor chains B should be
replaced by $\frac{zB}{2}$. What is physically happening is that the correlation length
on each chain is increasing as temperature is lowered until the average
number of bonds in each ordered region times the interaction energy per bond
with neighboring chains is larger than the thermal energy.[13] For temperatures
below this the chains are locked together too strongly to be broken by thermal
fluctuations.

It is interesting to note that the three dimensional ordering temperature
T_c is usually below the one-dimensional mean field transition T_{MF} (by a
factor of about $\ell n \, (\frac{2V_o}{B})$). We expect the transitions to have the general
behavior shown in figure 12. As temperature is lowered through T_{MF} we form
some bonds, the crystal distorts and charge density waves appear in isolated
regions. The amplitude of the displacements and charge density waves increase
as we get cooler, but the prevalent effect is the growth of the size of the

ordered regions or correlation length. Finally the chains order three dimensionally at T_c at which temperature the gap, charge density and distortions are essentially fully developed.

Conclusion

We have seen that one-dimensional metals are quite generally unstable against the formation of an insulating distorted state at low temperatures and that the problem associated with one-dimensional phase transitions is overcome by the three-dimensional nature of most physically realizable crystals.

How these ideas apply to the crystals under discussions at this conference depends strongly on the values of the different parameters and may vary widely. If coupling between chains is large the region between T_{MF} and T_c may be too small to be physically significant. If the electron-lattice coupling is small then T_{MF} may be reduced to a low enough temperature that other interactions predominate. Nonetheless, there is ample experimental evidence that these effects have been seen in several compounds[14,15] and we will doubtless find even more fascinating properties as new compounds continue to be synthesized. There are in addition many other related instabilities which are possible in one-dimensional metals including a Mott-Hubbard or magnetic insulator transition[16] and superconductivity.[17]

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Figure Captions

I. Density response of a uniformly dense electron gas in the presence of
    a periodic potential of wavevector q and amplitude V_o.

II. The response function or Lindhard function for a one-dimensional and
     three-dimensional electron gas. The solid lines are for zero temperature
     while the dashed lines represent non-zero temperature.

III. The results of quantum mechanical perturbation theory. a) In second
     order perturbation theory energy levels which are coupled by the perturbation
     repel. b) If states with the same energy are coupled, they are split by the
     coupling energy.

IV. The Fermi surfaces of a free electron gas. a) For three dimensions all
     states with $|\vec{k}| < k_F$ are occupied. For a given perturbation of wave-
     vector q only two equal energy states on the Fermi surface are coupled.
     b) For one dimension all states with $|k_x| < k_F$ are occupied. A perturbation
     of wavevector $q = 2k_F$ couples a set of planes of degenerate states on
     the Fermi surface.

V. For a three-dimensional Fermi surface regions may "nest." For tight binding
    bands with one electron per unit cell the wavevector $q = (\,^{\pi}/a_1,\quad ^{\pi}/b_1,\quad ^{\pi}/c\,)$
    always brings one part of the Fermi surface into juxtaposition with another
    part.

VI. If the ions in a crystal are periodically displaced the electrons respond
     by setting up a charge density wave.

VII. The solid line represents the natural frequencies of the lattice vibrations
     of a crystal. The dashed lines represent the lowering of the frequency of
     the lattice vibration at $q = 2k_F$ caused by the response of the electrons,
     known as the Kohn anomaly. As temperature is lowered the frequency is
   lowered.

VIII.   The solid line is the energy vs. wavevector (or momentum) of electrons in
        a metal. The arrows indicate the energy shifts when a periodic potential
        of wavevector q is applied.

IX.   The solid lines are the energy vs. wavevector of electrons in a metal
        after a potential of the form $V_o \cos \vec{q} \cdot \vec{r}$ has been applied. Note the energy
        gap at $k = q/2$. The shaded area is the lowering of the energy experienced
        by the electrons with $|k| < q/2$.

X.   The electrons effected by the periodic potential $V_o \cos \vec{q} \cdot \vec{r}$ are represented
        by the shaded area in a) and b). The fraction of electrons effected is
        larger in one dimension a) than in two dimensions b).

XI.   In a) we illustrate the undistorted, lattice with a uniform charge density.
        In b) a lattice distortion and charge density wave are illustrated in a
        fully ordered phase, corresponding to the lowest energy configuration.   In
        c) the order has been broken by skipping a bond at site i. The next ion
        has moved away from i and formed a separate bond rather than bonding with
        the ion at i.

XII.   The amplitude of the distortion or energy gap is shown as a function of
        temperature. The outer curve is the result of "mean field theory." However
        the actual phase transition to an ordered phase occurs at T_c 3-dim. where
        the interaction energy between chains is larger than the thermal energy.

XIII.   When interactions between chains are important the charge density waves
        arrange themselves so that positive and negative regions are adjacent in
        nearest neighbor chains. a) We represent this Coulomb interaction energy by
        -B when a bond is adjacent to an antibond and +B when bond is adjacent to
        bond or antibond to antibond. b) If one chain has a broken order,
        with a bond missing, then the rest of the chain (to the right of the break)
        experiences repulsive interactions for the remainder of its length.

Initial density

$\rho(r)$ ρ_0

r →

Periodic potential

$V(r) = V_0 \cos \vec{q} \cdot \vec{r}$

$V(r)$

V_0

0

$-V_0$

$\frac{2\pi}{q}$

r →
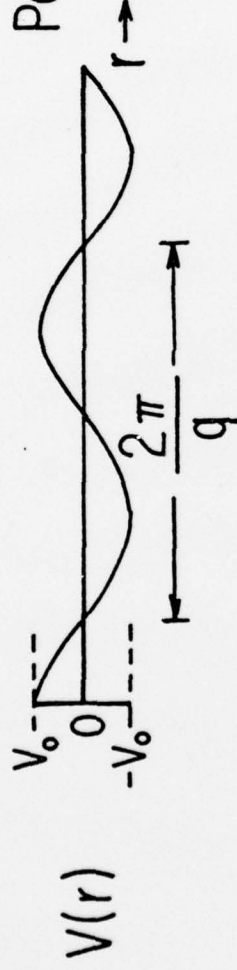
Density in presence of potential

$\rho(r)$

ρ_0

r →

Density response to periodic potential

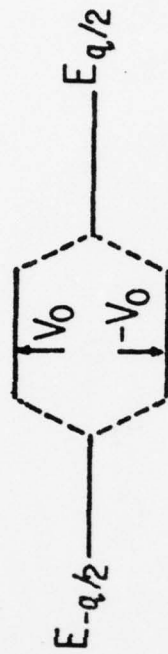$\delta\rho(r) = X(q) V_0 \cos \vec{q} \cdot \vec{r}$

$\delta\rho(r)$

$V_0 x(q)$

r →
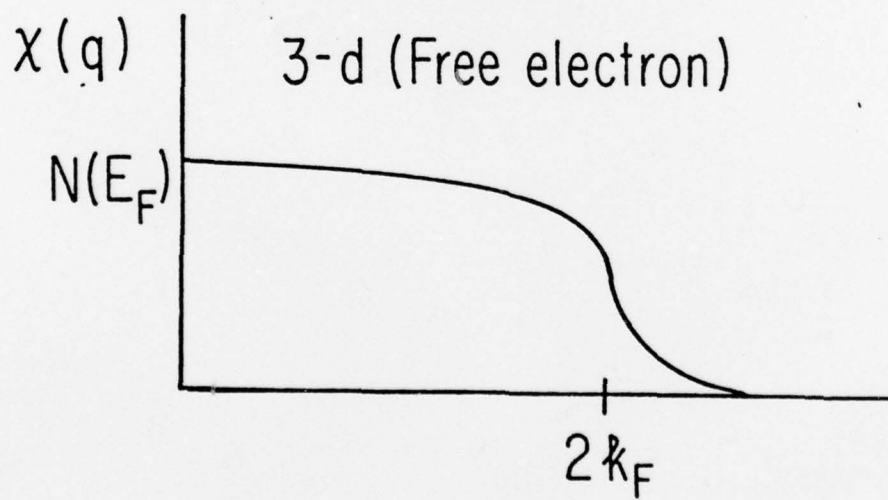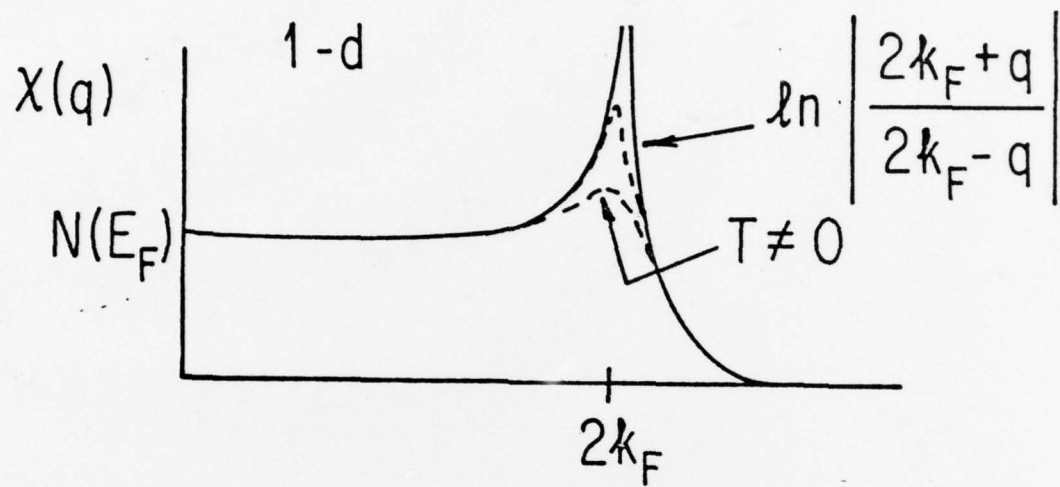
2nd order perturbation theory

Degenerate perturbation theory

E_{k+q}

E_k

$$\frac{V_0^2}{E_k - E_{k+q}}$$

$$\frac{V_0^2}{E_{k+q} - E_k}$$

a)

$E_{-q/2}$

$E_{q/2}$

V_0

$-V_0$

b)

1 dimension

3 dimensions

Degenerate states

k_y k_x k_F

$q = 2k_F$

k_y k_x k_F q
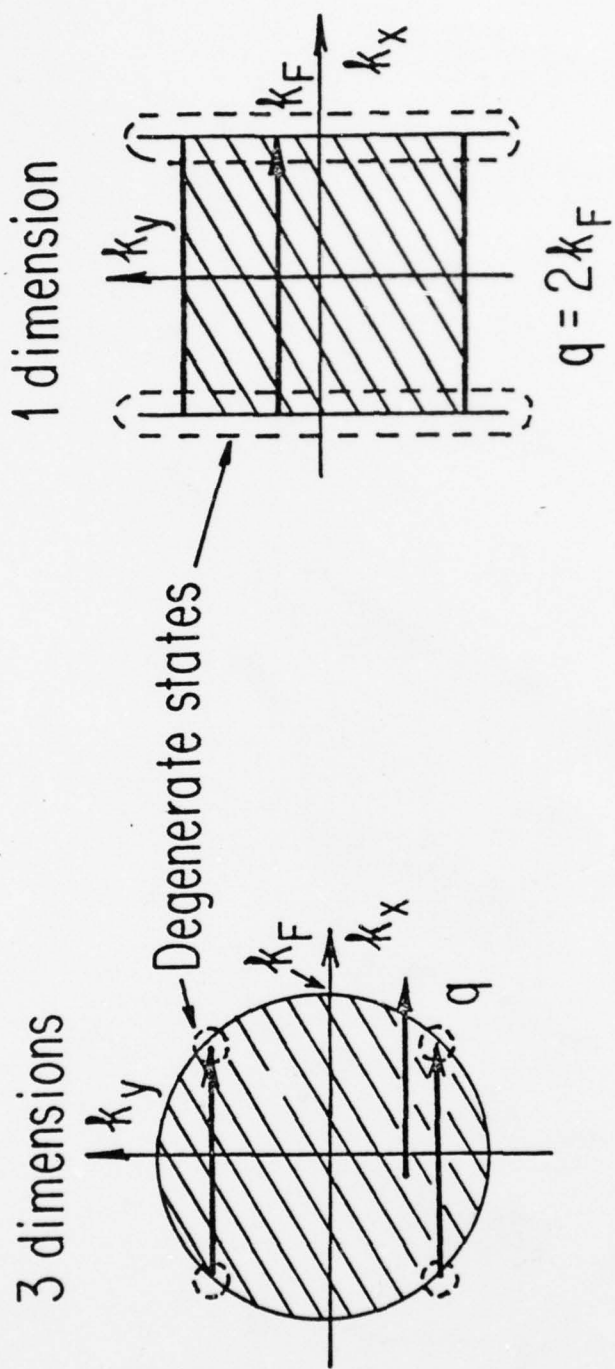
$\tau_x \neq \tau_y$

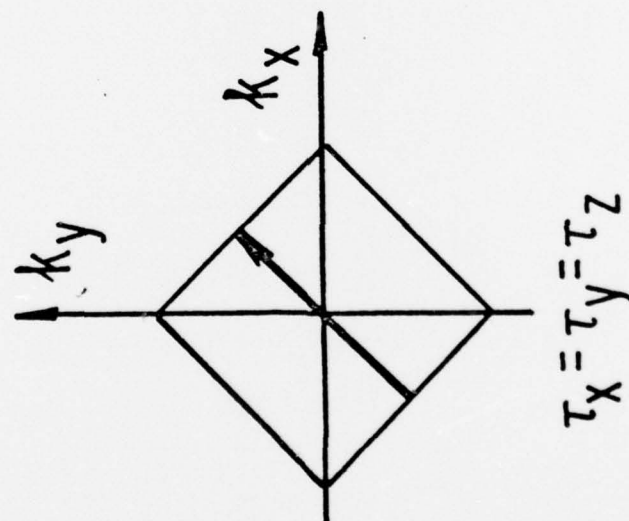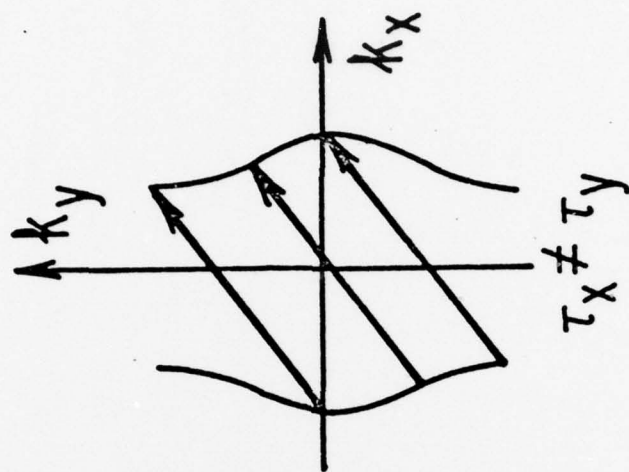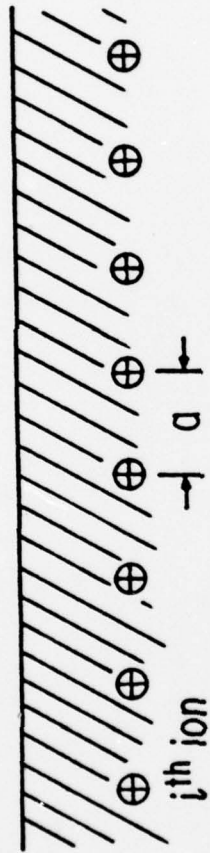$\tau_x = \tau_y = \tau_z$

$q = \dfrac{\pi}{a}, \dfrac{\pi}{b}, \dfrac{\pi}{c}$

Initial Configuration

Uniform neg. charge

Positive Ions

i^{th} ion

a

After periodic displacement

Charge density X_q g U_q

With displacement U_q

U_i

$2\pi/q$

1-dim

k_y

αV_0

k_x

$q=2k_F$

a)

2-dim

k_y

αV_0

k_x

$q=2k_F$

b)

a) Uniform chain

b) Ordered phase with charged density wave

c) Order broken

missing "bond"